
MATLAB Functions for the Extraction of Refractive Indices from Aerosol Extinction Spectra

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Abstract

A set of functions has been developed in MATLAB to retrieve refractive indices from aerosol particle extinction spectra with the classical damped harmonic oscillator model. The aerosols are assumed to be spherical so that Mie theory can be applied to calculate the extinction efficiency and its derivatives. The particle size distribution is lognormal but can be easily adapted to other forms of distributions. The retrieved parameters are the particle distributions mean radius r_m , the standard deviation σ , the dielectric constants at high frequency ϵ'_∞ , and the classical damped harmonic oscillator band parameters, from which the refractive indices can be calculated. As a test, we extract the refractive indices of water ice and the particle size distributions from an extinction spectrum in the mid infrared region.

1 Introduction

It is often desired to retrieve the wavelength dependent optical constants of aerosol particles from their spectra. The optical constants that we are interested in are the refractive indices m_v ($m_v = n_v + ik_v$), the dielectric constant ϵ_v ($\epsilon_v = \epsilon'_v + i\epsilon''_v$), and the polarizability α_v ($\alpha_v = \alpha'_v + i\alpha''_v$). The relations between these optical constants are:¹

$$\epsilon_v = m_v^2, \epsilon'_v = n_v^2 - k_v^2, \epsilon''_v = 2n_vk_v \quad (1)$$

The polarizability is related to the dielectric constant (and refractive index) by the Lorentz-Lorentz relation ¹

$$\alpha_v = \left(\frac{\epsilon_v - 1}{\epsilon_v + 2} \right) \quad (2)$$

$$\epsilon_v = \left(\frac{1 + 2\alpha_v}{1 - \alpha_v} \right) \quad (3)$$

Here α_v (unitless) should be understood as the polarizability of a sphere with radius r divided by $4\pi r^3$. (ref 1, p139)

The real and imaginary parts of optical constants are interdependent. If one knows the imaginary part, the real part can be calculated using the Kramer-Kronig relations. Take the dielectric constants as an example,

$$\dot{\varepsilon}(\nu_l) = \varepsilon_\infty + \frac{2}{\pi} P \int_0^\infty \frac{\nu \ddot{\varepsilon} d\nu}{\nu^2 - \nu_l^2} \quad (4)$$

where P denotes the Cauchy principal value, and ε_∞ is the real part of dielectric constant at infinite frequency.¹

When the particles are small, the optical constant retrievals are simple; here, the total particle volume is important but not the specific size. Also, the imaginary part of polarizability is proportional to the extinction.² When particles are large, the retrievals become complicated because both parts of refractive indices should be considered, as well as the specific sizes. Thomas³⁻⁴ *et al.* introduced the classical damped harmonic oscillator (CDHO) model based retrieval method where they use the CDHO bands parameters, along with Mie theory to simulate the extinction spectrum and then fitted to the measured spectra. Employing this retrieval method, both parts of refractive indices as well as the size distribution can be extracted from a single extinction spectrum.^{3, 5} In the following sections, basic formulas relevant to the retrieval will be introduced.

2 Formulas

2.1 The classical damped harmonic oscillator

The complex dielectric constant and polarizability of a material can be expressed as a function of band parameters using classical damped harmonic oscillator model.⁶ In the CDHO model, if the j^{th} oscillator intensity is S_j (cm^{-2}), the damping constant is γ_j (cm^{-1}), and the band position is $\tilde{\nu}_j$ (cm^{-1}) then the dielectric constants are

$$\ddot{\varepsilon}(\tilde{\nu}_l) = \sum_j \frac{S_j \gamma_j \tilde{\nu}_l}{(\tilde{\nu}_j^2 - \tilde{\nu}_l^2)^2 + \gamma_j^2 \tilde{\nu}_l^2} \quad (5)$$

$$\dot{\varepsilon}(\tilde{\nu}_l) = \varepsilon_\infty + \sum_j \frac{S_j (\tilde{\nu}_j^2 - \tilde{\nu}_l^2)}{(\tilde{\nu}_j^2 - \tilde{\nu}_l^2)^2 + \gamma_j^2 \tilde{\nu}_l^2} \quad (6)$$

where ε_∞ is the real part of dielectric constant at infinite frequency.

2.2 The Extinction Spectra for an Ensemble of Particles

For homogeneously distributed aerosols, if input irradiance is I_0 , transmitted irradiance is I_t , and the optical path is L , then the extinction spectrum A is⁷

$$A = -\ln\left(\frac{I_t}{I_0}\right) \cong \sum NLP(r)Q(x,m)\pi r^2 dr \quad (7)$$

where N (particles / cm³) is total particle number density, $P(r) dr$ is population fraction of particles of radius between r and $r + dr$, $Q(x_i, m_l)$ is the extinction efficiency which depends on the complex refractive index m_l and size parameter $x_i = 2\pi r_i \tilde{\nu}$, where $\tilde{\nu}$ is the wavenumber, i.e. the inverse of the wavelength. Note the right side of the equation (7) is approximation of the integral over continues size distribution as summation over discrete size bins. The validity of this approximation can be checked by adding $P(r)dr$ over the whole size distribution which should be close to 1. For clarity, A can be expressed in matrix notation as:

$$A = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_l \end{bmatrix} = \pi N L d r \begin{bmatrix} Q(x_1, m_1) & Q(x_2, m_1) & \dots & Q(x_g, m_1) \\ Q(x_1, m_2) & Q(x_2, m_2) & \dots & Q(x_g, m_2) \\ \vdots & \vdots & \ddots & \vdots \\ Q(x_1, m_l) & Q(x_2, m_l) & \dots & Q(x_g, m_l) \end{bmatrix} \begin{bmatrix} P(r_1) r_1^2 \\ P(r_2) r_2^2 \\ \vdots \\ P(r_g) r_g^2 \end{bmatrix} \quad (8)$$

In equation (8), the only parameter that depends on refractive indices is the extinction efficiency Q . Assuming all other factors are known, then Q can be easily inferred. But here we are interested in extracting the refractive indices. We do so by employing the CDHO based approach.

2.3 The Lognormal Distribution

We assume the particles' size is log normal distributed around mean radius r_m with standard deviation σ , then we have ⁴

$$P(r) = \frac{1}{\sqrt{2\pi} r \ln \sigma} \exp \left[-\frac{1}{2} \left(\frac{\ln(r/r_m)}{\ln \sigma} \right)^2 \right] \quad (9)$$

Here mean radius r_m and standard deviation σ are with respect to the distribution of $\ln(P)$ which is normal distribution

2.4 The CDHO based Retrieval

In the method, one starts with an initial 'guessed' CDHO band parameters from which the dielectric constants, and hence the refractive indices, can be calculated. Then using this 'guessed' refractive indices, along with the size distribution and other parameters in equation (7), an extinction spectrum can be calculated. In the next step, the CDHO band parameters or other unknowns are iteratively improved. This is achieved by minimizing the sum of residual squares, χ^2 , between calculated extinction spectra A^{Mie} and experimental spectra A , i.e.

$$\chi^2 = \sum_{i=1}^l (\Delta A_i)^2, \quad \Delta A_i = A_i^{Mie} - A_i \quad (10)$$

It is worth pointing out that in the fitting of spectra to equation (7), the product of particle concentration N and path length L is just a scaling factor, if not known, it can be set to a value where the simulated spectra matches the experimental one at a certain wavenumber. The χ^2 can be minimized using various non-linear least-square optimization techniques, like the well-known Levenberg-Marquardt algorithm. Matlab also provides the trust-region-reflective algorithm (an evolution of Levenberg-Marquardt algorithm) on solving non-linear least-square problems,⁸ which we employ here. The MATLAB function *lsqnonlin* (*fun*,*x0*,*lb*,*ub*,*options*), which is called for the minimization of χ^2 , requires the input function to be minimized (χ^2 here, equation (10)) the initial values of the parameters to be optimized (*par*, equation (14)), the lower (*lb*) and upper bounds (*ub*) of the parameters, and the options that control the implementation of algorithm. The options can be set using *options=optimoptions()* where the algorithm (here, trust-region-reflective) and the convergence criteria can be chosen, as well as how the Jacobian (the extinction derivative matrix) to be calculated, numerical or analytical. We provide the analytical Jacobian, as discussed by Grainger et al^{3,4} and in the following sections.

2.5. The Derivatives

Just considering CDHO band parameters, we can express as the total differentiation of extinction A with respect to CDHO band parameters in a matrix form:

$$\begin{bmatrix} \Delta A_1 \\ \Delta A_2 \\ \vdots \\ \Delta A_l \end{bmatrix} = \begin{bmatrix} \frac{\partial A_1}{\partial v_1} & \frac{\partial A_1}{\partial S_1} & \frac{\partial A_1}{\partial \gamma_1} & \frac{\partial A_1}{\partial v_2} & \frac{\partial A_1}{\partial S_2} & \frac{\partial A_1}{\partial \gamma_2} & \dots & \frac{\partial A_1}{\partial v_j} & \frac{\partial A_1}{\partial S_j} & \frac{\partial A_1}{\partial \gamma_j} \\ \frac{\partial A_2}{\partial v_1} & \frac{\partial A_2}{\partial S_1} & \frac{\partial A_2}{\partial \gamma_1} & \frac{\partial A_2}{\partial v_2} & \frac{\partial A_2}{\partial S_2} & \frac{\partial A_2}{\partial \gamma_2} & \dots & \frac{\partial A_2}{\partial v_j} & \frac{\partial A_2}{\partial S_j} & \frac{\partial A_2}{\partial \gamma_j} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ \frac{\partial A_l}{\partial v_1} & \frac{\partial A_l}{\partial S_1} & \frac{\partial A_l}{\partial \gamma_1} & \frac{\partial A_l}{\partial v_2} & \frac{\partial A_l}{\partial S_2} & \frac{\partial A_l}{\partial \gamma_2} & \dots & \frac{\partial A_l}{\partial v_j} & \frac{\partial A_l}{\partial S_j} & \frac{\partial A_l}{\partial \gamma_j} \end{bmatrix} \begin{bmatrix} \Delta v_1 \\ \Delta S_1 \\ \Delta \gamma_1 \\ \Delta v_2 \\ \Delta S_2 \\ \Delta \gamma_2 \\ \vdots \\ \Delta v_j \\ \Delta S_j \\ \Delta \gamma_j \end{bmatrix} \quad (11)$$

If other parameters are to be optimized, then they can be arranged in similar way. For now, we just consider the CDHO band parameters. The first column of the extinction derivative matrix (the first part of right side of equation (11)) can be expressed as:

$$\begin{bmatrix} \frac{\partial A_1}{\partial v_1} \\ \frac{\partial A_2}{\partial v_1} \\ \vdots \\ \frac{\partial A_l}{\partial v_1} \end{bmatrix} = \pi N L d r \begin{bmatrix} \frac{\partial Q_{11}}{\partial v_1} & \frac{\partial Q_{12}}{\partial v_1} & \dots & \frac{\partial Q_{1g}}{\partial v_1} \\ \frac{\partial Q_{21}}{\partial v_1} & \frac{\partial Q_{22}}{\partial v_1} & \dots & \frac{\partial Q_{2g}}{\partial v_1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial Q_{l1}}{\partial v_1} & \frac{\partial Q_{l2}}{\partial v_1} & \dots & \frac{\partial Q_{lg}}{\partial v_1} \end{bmatrix} \begin{bmatrix} P(r_1)r_1^2 \\ P(r_2)r_2^2 \\ \vdots \\ P(r_g)r_g^2 \end{bmatrix} \quad (12)$$

The other columns of the derivative matrix can also be calculated in a similar way. The derivatives of extinction efficiencies with respect to the CDHO band parameters are given as:³

$$\frac{\partial Q_{lg}}{\partial v_1} = \frac{\partial Q_{lg}}{\partial k_1} \frac{\partial k_1}{\partial v_1} + \frac{\partial Q_{lg}}{\partial n_1} \frac{\partial n_1}{\partial v_1} \quad (13)$$

The derivatives of extinction efficiencies Q with respect to the refractive indices k and n are given by Gaigener,⁴ and the derivatives of refractive indices k and n with respect to the CDHO band parameters are given in reference³ by the same author. Note the units of the Jacobians (the extinction derivative matrix) can be deduced from equation (11) and (14), where the first j columns are [cm cm² cm ... cm cm² cm], the next column is the extinction derivative with respect to ϵ_∞ which is unitless, the next two columns are extinction derivatives with respect to the size distribution parameters r_m and σ (the derivative units are cm⁻¹ and 1, respectively) followed by the extinction derivative with respect to the column density NL (derivative units cm² / particle).

3. The MATLAB Programs

These MATLAB codes are written and tested on MATLAB R2014B version running on 64 bit Windows 7 PC. The code is accelerated using the MATLAB Parallel Computing toolbox, with the key word ‘parfor’. If not needed, the keyword can be changed to ‘for’ but the speed would be very slow. The keyword ‘parpool (‘local’,3)’ invokes the Parallel Computing toolbox on local machine and runs on 3 cores.

All the codes have been written by Mahmut Ruzi, except me_ab_deriv and mie_q_deriv which were originally written by Christian Mätzler⁹ in 2002. The original codes have been extended by Mahmut Ruzi to also compute the derivatives.

3.1 The function opt_cdhopar.

This is the main function used for the least squares minimization. The particle size distribution is assumed to be lognormal. The outputs from this function are the residuals, and

the Jacobians. The inputs are the extinction spectra sp and wavenumber v (column vectors, units cm^{-1}), the particle size row vector r (cm), and the matrix par to be defined. If the number of CDHO bands is j , then par is organised as:

$$par = \begin{bmatrix} v_1 & v_2 & \cdots & v_j & \epsilon'_\infty & NL \\ S_1 & S_2 & \cdots & S_j & r_m & 1 \\ \gamma_1 & \gamma_j & \cdots & \gamma_j & \sigma & 1 \end{bmatrix} \quad (14)$$

Here the first j columns are the CDHO band parameters, ϵ'_∞ is the real part of dielectric constant at infinite frequency, r_m is the lognormal distribution mean size, and σ is its standard deviation. In the last column, NL is the product of optical path length and particle total number concentration (see equation 7), and the last two ‘ones’ are just dummy numbers. Note that the form of the Jacobian is the same as in equation (11). In the following sections, the main function and its related sub-functions are listed.

The function `opt_cdhopar`:

```
function [res,jacres] = opt_cdhopar(par,sp,v,r)
    dr=abs(r(2)-r(1));
    P=lognpdf(r,par(2,end-1),par(3,end-1));
    ps=dr*(P.*r.*r)';
    x=2*pi*v*r; % size parameter
    nl=par(1,end);
    %%
    [ei,erl]= cdho(v,par(:,1:end-2));
    er_inf=par(1,end-1);
    er=er_inf+erl;
    % refractive indices
    m=sqrt(er+1i*ei);
    M=m*ones(1,size(x,2));
    Q=zeros(size(x)); Qdermr=Q; Qdermi=Q;
    parfor w=1:size(x,1)*size(x,2)
        [Q(w),~,Qdermr(w),Qdermi(w)]=mie_q_deriv(M(w),x(w));
    end

    %%
    res=(pi*nl*Q*ps-sp).*1);

    %% Jacobian

    if nargin>1
        dqdpar= qextderiv_cdhopar(par(:,1:end-2),v,par(1,end-1),Qdermi,Qdermr);
        [dnder,~,dkder,~]= refindxderiv_e(ei,er);

        dqder_inf=Qdermr.*(dnder*ones(1,size(x,2)))+Qdermi.*(dkder*ones(1,size(x,2))));

        jcdho=pi*nl*dqdpar*ps;
        jer_inf=pi*nl*dqder_inf*ps;
        % size distribution derivatives
        [dpdmu,dpdsigma]=sizepderiv(r,par(2,end-1),par(3,end-1));
        jacsizemu=pi*nl*Q*((dr*dpdmu.*r.*r)');
```

```

        jacsizesig=pi*n1*Q*((dr*dpdsigma.*r.*r)');
        jacres=[reshape(jcdho,length(v),numel(par(:,1:end-2))) jer_inf ...
            jacsizemu jacsizesig pi*Q*ps zeros(length(v),2)];
    end
    %%
    function dqdpar= qextderiv_cdhopar(par,v,er_inf,dqdk,dqdn)
        [dkdpar,dndpar]=refracindx_deriv(v,par,er_inf);
        dkdpar=reshape(dkdpar,length(v)*numel(par),1)*ones(1,size(dqdk,2));
        dndpar=reshape(dndpar,length(v)*numel(par),1)*ones(1,size(dqdk,2));

    dqdpar=repmat(dqdk,numel(par),1).*dkdpar+repmat(dqdn,numel(par),1).*dndpar;
    end
    %%
    function [dpdmu,dpdsigma] = sizeparderiv(x,mu,sigma)
        % this function calculates first derivative of lognormal
distribution function with
        % respect to mu and sigma.

        dpdmu=(lognpdf(x,mu,sigma).*(log(x)-mu))./(sigma.^2);
        dpdsigma=(lognpdf(x,mu,sigma).*((log(x)-mu).^2))./(sigma.^3)-...
            lognpdf(x,mu,sigma)./(sigma);
    end

end

```

The function cdho:

```

function [alpha_i,alpha_r]= cdho(V,par0)
% classical damped harmonic oscillator model
% see J.E.Bertie and S.L. Zhang,Can.J.chem.70(1992),520
% input: v wavelength range,vj and gama_j are peak positions and damping
% constants, respectively
% output: real and imaginary refractive indices
% V is column matrix, Vj,Sj,and Gamma_j is row matrix
V0=par0(1,:);Vp=par0(2,:);sigma=par0(3,:);
v=V*ones(1,length(V0));vj=ones(length(V),1)*V0;vp=ones(length(V),1)*Vp; %
vectorise
sigma=ones(length(V),1)*sigma; % vectorise
t0=(vj.^2-v.^2);
t1=sigma.*v;
t2=vp./((t0).^2+(t1).^2);
aj=(t2.*t1);
alpha_i=sum(aj,2);
ajr=(t2.*t0);
alpha_r=sum(ajr,2);
end

```

The function mie_q_deriv:

```

function [result1,result2,qdermr,qdermi]= mie_q_deriv(m, x)

% Computation of Mie Efficiencies for given

```

```

% complex refractive-index ratio m=m'+im"

% and size parameter x=k0*a, where k0= wave number in ambient
% medium, a=sphere radius, using complex Mie Coefficients

% an and bn for n=1 to nmax,

% s. Bohren and Huffman (1983) BEWI:TDD122, p. 103,119-122,477.

% Result: m', m", x, efficiencies for extinction (qext),
% scattering (qsca), absorption (qabs), backscattering (qb),
% asymmetry parameter (asy=<costeta>) and (qratio=qb/qsca).

% Uses the function "Mie_ab" for an and bn, for n=1 to nmax.

% C. Mätzler, May 2002, revised July 2002.

% The original code of C. Mätzler is extended to calculate the Mie
% derivative, which are calculated using the relations in the paper by
% R.G.Grainger et al. Calculations of Mie Derivatives, Applied Optics,
% 43(2004),5386-5393

% Mahmut Ruzi, November 2017

if x==0                                % To avoid a singularity at x=0

    result1=[0 0 0 0 0 1.5];
    result2=[0 0 0 0 0 1.5];

elseif x>0                             % This is the normal situation

    nmax=round(2+x+4*x.^(1/3));

    % n1=nmax-1;

    n=(1:nmax);cn=2*n+1; % c1n=n.*(n+2)./(n+1); c2n=cn./n./(n+1);

    x2=x.*x;

    f=mie_ab_deriv(m,x);

    anp=(real(f(1,:)));  anpp=(imag(f(1,:)));

    bnp=(real(f(2,:)));  bnpp=(imag(f(2,:)));
    % efficiency derivatives
    anbnderrsum=real(f(3,:)+f(5,:));    % R.G.Grainger eq.(27)
    anbnderisum=real(f(4,:)+f(6,:));    % R.G.Grainger eq.(28)
%
    dn=cn.*(anp+bnp);

    q=sum(dn);

    qext=2*q/x2;

```

```

    % extinctin efficiency derivatives
    qdermr=-2*sum(cn.*anbnderrsum)/x2;    % R.G.Grainger eq.(27)
    qdermi=-2*sum(cn.*anbnderisum)/x2;    % R.G.Grainger eq.(28)
% Note the sign of the above two (qdermr and qdermi) are opposite of the
% original paper. The sign change is done to get the same results as the
numerical derivatives.
% We believe the equations on the paper are typographical mistakes.
    en=cn.*(anp.*anp+anpp.*anpp+bnp.*bnp+bnpp.*bnpp);

    q=sum(en);

    qsca=2*q/x2;

    result1=qext;result2=qsca;

end;

```

The function mie_ab_deriv

```

function result = mie_ab_deriv(m,x)

% Computes a matrix of Mie Coefficients, an, bn, and its derivatives w.r.t
% real and imaginary part of refractive indices.

% of orders n=1 to nmax, for given complex refractive-index

% ratio m=m'+im" and size parameter x=k0*a where k0= wave number in ambient
% medium for spheres of radius a;

% Eq. (4.88) of Bohren and Huffman (1983), BEWI:TDD122

% using the recurrence relation (4.89) for Dn on p. 127 and

% starting conditions as described in Appendix A.

% C. Mätzler, July 2002
% The original code of C. Mätzler is extended to calculate the mie
% derivative, which are calculated using the relations in the paper by
% R.G.Grainger et al. Calculations of Mie Derivatives, Applied Optics,
% 43(2004),5386-5393
% Mahmut Ruzi, November 2017

z=m.*x;

nmax=round(2+x+4*x.^(1/3));

nmx=round(max(nmax,abs(z))+16);

n=(1:nmax); nu = (n+0.5);

```

```

sx=sqrt(0.5*pi*x);

px=sx.*besselj(nu,x);

plx=[sin(x), px(1:nmax-1)];

chx=-sx.*bessely(nu,x);

chl=[cos(x), chx(1:nmax-1)];

gsx=px-li*chx; gslx=plx-li*chl;

dnx(nmx)=0+0i;

for j=nmx:-1:2      % Computation of Dn(z) according to (4.89) of B+H
(1983)

    dnx(j-1)=j./z-1/(dnx(j)+j./z);

end;

dn=dnx(n);          % Dn(z), n=1 to nmax

da=dn./m+n./x;

db=m.*dn+n./x;

an=(da.*px-plx)./(da.*gsx-gslx);

bn=(db.*px-plx)./(db.*gsx-gslx);

% derivatives
andermr=li*(n.*(n+1)./z-z.*(1+dn.^2)-dn)/(((dn+n.*m./x).*gsx-m.*gslx).^2);
% R.G.Grainger eq.(41)
andermi=-(n.*(n+1)./z-z.*(1+dn.^2)-dn)/(((dn+n.*m./x).*gsx-m.*gslx).^2);
% R.G.Grainger eq.(42)

bndermr=li*(n.*(n+1)./z-z.*(1+dn.^2)+dn)/(((dn+n.*m./x).*gsx-m.*gslx).^2);
% R.G.Grainger eq.(44)

bndermi=-(n.*(n+1)./z-z.*(1+dn.^2)+dn)/(((dn+n.*m./x).*gsx-m.*gslx).^2);
% R.G.Grainger eq.(45)

result=[an; bn; andermr; andermi;bndermr;bndermi];

```

The function `refindxderiv_e`:

```

function [dnder,dndei,dkder,dkdei]= refindxderiv_e(ei,er)
%refractive index derivative with respect to dielectric constant
% input:  er - dielectric constant, real part

```

```

%      ei - dielectric constant, imaginary part
% output: dnder - real refractive index derivative wrt real dielectric
%           constant;
% other symbols are of similar meaning

dnder=(er./(2.*sqrt(ei.^2 + er.^2)) + 1/2)./(2.*sqrt(sqrt(ei.^2 + er.^2)./2
+ er./2));
%
dnder=er./sqrt((8*sqrt(er.^2+ei.^2)+er).*(er.^2+ei.^2))+1./sqrt(8*sqrt(er.
^2+ei.^2));
dndei=ei./(4.*sqrt(sqrt(ei.^2 + er.^2)./2 + er./2).*sqrt(ei.^2 + er.^2));

dkder=(er./(2.*sqrt(ei.^2 + er.^2)) - 1/2)./(2.*sqrt(sqrt(ei.^2 + er.^2)./2
- er./2));
dkdei=ei./(4.*sqrt(sqrt(ei.^2 + er.^2)./2 - er./2).*sqrt(ei.^2 + er.^2));
end

```

The function refracindx_deriv

```

function [dkdpar,dndpar] =refracindx_deriv(v,par,er_inf)
% [dkdpar,dndpar] =refracindx_deriv(v,par)
% refractive index derivatives w.r.t dielectric CDHO parameters;
% input ---v: w by 1 column vectore, wavenumber;
%      ---par: 3 by g CDHO parameters, format [v1 v2 ...vg;
%              s1 s2 ...sg;
%              y1 y2 ...yg];
%              where v1 is band position, s1 is intensity, and y1 is width
%      ---er_inf: real dielectric constant at infinite frequency

% output ---dkdpar: imaginary refractive indices derivatives w.r.t CDHO
parameters,
%      ---dndpar: real refractive indices derivatives w.r.t CDHO
parameters
%              both are w by 3*g matrix;
%              format:[dk1dv1 dk1ds1 dk1dy1 dk1dv2 dk1ds2 dk1dy2 ...;
%              dk2dv1 dk2ds1 dk2dy1 dk2dv2 dk2ds2 dk2dy2 ...
%              .      .      .      .      .      .
%              dkwdv1 dkwds1 dkwdy1 dkwdv2 dkwds2 dkwdy2 ...]

% written by Mahmut Ruzi, La Trobe Insitue for Molecular Sciences, La Trobe
% University, Melbourne, Australia, July 2016

[ei,er,aider,arder] = cdhoderiv(v,par);
er=er+er_inf;
t0=sqrt(ei.^2 + er.^2);
dnder=(er./(2.*t0) + 1/2)./(2.*sqrt(t0./2 + er./2));
dndei=ei./(4.*sqrt(t0./2 + er./2).*t0);

dkder=(er./(2.*t0) - 1/2)./(2.*sqrt(t0./2 - er./2));
dkdei=ei./(4.*sqrt(t0./2 - er./2).*t0);

dkdpar=aider.*(dkdei*ones(1,numel(par)))+arder.*(dkder*ones(1,numel(par)));
dndpar=aider.*(dndei*ones(1,numel(par)))+arder.*(dnder*ones(1,numel(par)));

end

```

Examples and Tests

One can test the code by running the `spec2nk_demo` file. It loads an extinction spectrum of water ice and ‘guessed’ 16 CDHO bands to fit the spectrum, and retrieve the optimised CDHO and size distribution parameters, as well as ε_{∞} . The fitting results are shown in

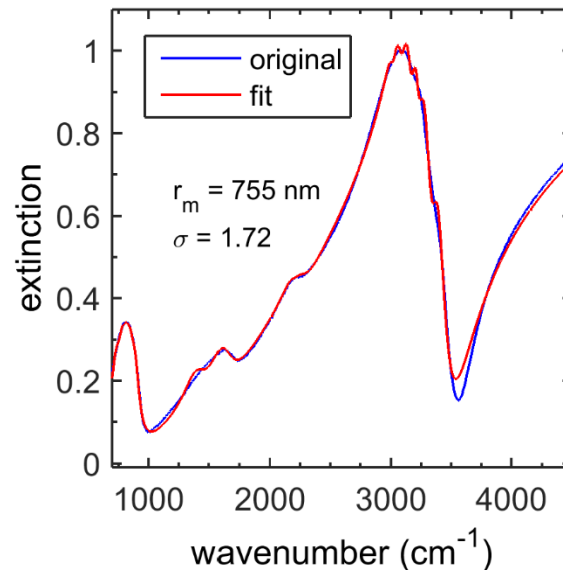


Figure 1. The original and fitted extinction spectra of water ice in the mid infrared region. The particles are assumed to be lognormal distributed, and the optimised mean size r_m and standard deviation σ are also shown.

figure 1, and the refractive indices are shown in figure 2.

It is clear from figure 1 and 2 that the results of the fitting is reasonable, even if the input refractive indices (or CDHO band parameters) are very different from the optimal values. For extended tests, refer to the thesis⁵ by one of the authors.

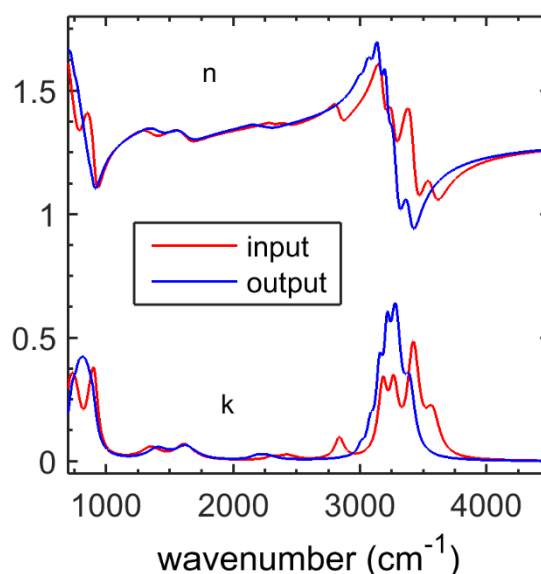


Figure 2. The input and optimised refractive indices, calculated using the CDHO band parameters.

Conclusion

A set of MATLAB codes have been written to retrieve refractive indices, as well as size distribution parameters from a single extinction spectrum of aerosol particles. The main idea of the method is to use classical damped harmonic oscillator model to simulate the refractive indices, and the Mie theory to simulate extinction, and then fit it to the measured extinction employing some least square methods. The codes have been tested on water ice to retrieve refractive indices and size distribution parameters from ice aerosol particles extinction spectra.

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